

Supercriticality and Transmission Resonances in the Dirac Equation

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It is shown that a Dirac particle of mass m and arbitrarily small momentum will tunnel without reflection through a potential barrier $V = U_c(x)$ of finite range provided that the potential well $V = -U_c(x)$ supports a bound state of energy $E = -m$. This is called a supercritical potential well.

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It is now over 70 years since the Dirac equation was written down. Yet new results have been discussed in recent years, even in the relatively simple cases of one [1] and two spatial dimensions [2] as well as in three dimensions [3]–[6]. In this note, we generalise a well known theorem of scattering off a one-dimensional potential well in the Schrödinger equation to the Dirac equation. This is not difficult, but the theorem has an unexpected twist. Since the Dirac equation covers anti-particle scattering as well as particle scattering, the generalisation gives two distinct results. One of these results implies a remarkable property of tunnelling through a potential barrier in the Dirac equation which is related to the result on barrier penetration found by Klein [7] and now called the Klein Paradox.

We begin by considering the scattering off a class of one-dimensional potential wells $V(x)$ where $V(x) = 0$ for $|x| \geq a$ and $V(x) = -U(x) \leq 0$ for $|x| < a$ where the piecewise continuous function $U(x) \geq 0$. The potential is also taken to be even so that $V(-x) = V(x)$. We first seek to generalise to the Dirac equation the non-relativistic result that the reflection coefficient $R(k)$ for scattering off the potential well $V(x) = -U_0(x)$ which supports a zero energy resonance satisfies $R(0) = 0$, where k is the momentum of the particle. This theorem was known to Schiff [8] and Bohm [9] but a proof was published only relatively recently by Senn [10] and Sassoli de Bianchi [11]. The situation where $R(k) = 0$ and the transmission coefficient $T(k) = 1$ is called a transmission resonance [9]. In non-relativistic systems a zero energy resonance (or half-bound state) [12] is the non-trivial limit where a bound state just emerges from the continuum, for example when a square well potential is just strong enough to support a second bound state.

Following an earlier paper [13] we take the gamma matrices γ_x and γ_0 to be the Pauli matrices σ_x and σ_z respectively. Then the Dirac equation for scattering of a particle of energy E and momentum k by the potential $V(x)$ can be written as the coupled equations

$$\frac{\partial f}{\partial x} + (E - V(x) + m)g = 0 \quad (1a)$$

$$\frac{\partial g}{\partial x} - (E - V(x) - m)f = 0 \quad (1b)$$

where the Dirac spinor $\psi = \begin{pmatrix} f \\ g \end{pmatrix}$.

Eqs. (1) have simple solutions as $x \rightarrow \pm\infty$ where $V = 0$. In particular, the analogue of a zero energy resonance in the Schrödinger equation is a zero momentum resonance in the Dirac equation [2] where a particle of zero momentum has $E = m$ or an anti-particle has $E = -m$.¹ It is easy to see that the solution of Eq. (1) for $E = m$ and $V = 0$ appropriately normalised is $\psi = \begin{pmatrix} 2m \\ 0 \end{pmatrix}$ while the solution for $E = -m$ and $V = 0$ is $\begin{pmatrix} 0 \\ 2m \end{pmatrix}$. As in Ref. [13] we can now write down the solutions of Eq. (1) for a particle of momentum k as $x \rightarrow \pm\infty$ to obtain $\psi = \begin{pmatrix} E + m \\ -ik \end{pmatrix} e^{ikx}$ while an anti-particle of momentum k will have $\psi = \begin{pmatrix} ik \\ m - E \end{pmatrix} e^{-ikx}$.

We now set up the usual formalism for particle scattering by the potential $V(x)$ in the Dirac equation. We take the particle as incident from the left, so the amplitude for reflection $r(k)$ is defined through the spinor $\psi(x)$ as $x \rightarrow -\infty$

$$\psi(x) = \begin{pmatrix} E + m \\ -ik \end{pmatrix} e^{ikx} + r(k) \begin{pmatrix} E + m \\ ik \end{pmatrix} e^{-ikx} \quad (2)$$

while as $x \rightarrow \infty$

$$\psi(x) = t(k) \begin{pmatrix} E + m \\ -ik \end{pmatrix} e^{ikx} \quad (3)$$

In the Dirac equation [14] as for the Schrödinger equation with symmetric potentials [11], unitarity implies that

$$|r|^2 + |t|^2 = 1; \quad \text{Im}(r^*t) = 0 \quad (4)$$

so $R + T = 1$ where the reflection and transmission coefficients are given by $R = |r|^2$, $T = |t|^2$.

¹The anti-particle is described by the hole wave function corresponding to the absence of the state with $E = -m$

Since the potentials we consider are even, parity is conserved. In our two-component approach, the transformation of a wave function under $x \rightarrow -x$ is given [13] by

$$\psi'(x, t) = \sigma_z \psi(-x, t) \quad (5)$$

It follows that an even wave function ψ has an even top component f and an odd bottom component g . Similarly for an odd wave function ψ , f will be odd and g will be even.

We first consider an even bound state in the potential $V(x)$. As $x \rightarrow \pm\infty$, its unnormalised wave function will be of the form

$$\psi(x) = \begin{pmatrix} m+E \\ -\kappa \end{pmatrix} e^{\kappa x} \quad x \rightarrow -\infty \quad (6a)$$

$$\psi(x) = \begin{pmatrix} m+E \\ \kappa \end{pmatrix} e^{-\kappa x} \quad x \rightarrow \infty \quad (6b)$$

where $E^2 = m^2 - \kappa^2$. We require the potential well $V = -U_0(x)$ to just bind this bound state with arbitrarily small κ . If this is the case, then the limit $\kappa \rightarrow 0$ exists, and $\psi(x)$ becomes a continuum wave function since it is no longer square integrable.

We can now compare Eqs. (6) with Eqs (2) and (3) in the limit $k \rightarrow 0, \kappa \rightarrow 0$. We obtain $2m(1+r(0)) = 2mt(0)$ or

$$1 + r(0) = t(0) \neq 0 \quad (7)$$

We have written $t(0) \neq 0$ since otherwise $\psi(x)$ would vanish in the limit $k \rightarrow 0, \kappa \rightarrow 0$ and we would not be considering a zero momentum resonance.²

The theorem now follows easily just as it does in the Schrödinger case [11]. Combining Eq (7) with the unitarity condition $Im(r^*t) = 0$ of Eq (4), we get $Im(r^*) = 0$ so that $r(0)$ and $t(0)$ are real. From $|r|^2 + |t|^2 = 1$ we obtain

$$2r^2 + 2r + 1 = 1 \quad (8)$$

so that $r(0) = 0$ or $r(0) = -1$. Since $t(0) \neq 0$ we obtain the result $r(0) = 0$ and so in terms of the reflection and transmission coefficients

$$R(0) = 0 \quad T(0) = 1 \quad (9)$$

If instead we had considered an odd bound state, an additional minus sign must be introduced into either Eq. (6a) or Eq. (6b). Eq. (7) must be modified to $1 + r(0) = -t(0)$ and the subsequent analysis and conclusions remain valid. Hence just as in the Schrödinger

equation, the scattering of a particle in the Dirac equation off a potential well $V = -U_0(x)$ which “binds” a zero momentum resonance corresponds to a transmission resonance with zero reflection.

We now increase the strength of the potential well from $U_0(x)$ to $U_c(x)$ so that $V = -U_c(x)$ supports a bound state of energy $E = -m$. This is called a supercritical potential and is associated with spontaneous positron production [16], [17]. We can redo the analysis exactly as before by defining amplitudes r_-, t_- for the reflection and transmission of an anti-particle of momentum k incident from the left on a potential well $V(x)$: so in place of Eq. (2) we have as $x \rightarrow -\infty$

$$\psi(x) = \begin{pmatrix} ik \\ m-E \end{pmatrix} e^{-ikx} + r_-(k) \begin{pmatrix} -ik \\ m-E \end{pmatrix} e^{ikx} \quad (10)$$

while as $x \rightarrow \infty$, we have

$$\psi(x) = t_-(k) \begin{pmatrix} ik \\ m-E \end{pmatrix} e^{-ikx} \quad (11)$$

As before unitarity gives

$$|r_-|^2 + |t_-|^2 = 1; \quad Im(r_-^* t_-) = 0 \quad (12)$$

and the near-supercritical even bound state for $x \rightarrow \pm\infty$ is now

$$\psi(x) = \begin{pmatrix} -\kappa \\ m-E \end{pmatrix} e^{\kappa x} \quad x \rightarrow -\infty \quad (13a)$$

$$\psi(x) = - \begin{pmatrix} \kappa \\ m-E \end{pmatrix} e^{-\kappa x} \quad x \rightarrow \infty \quad (13b)$$

Note again that for the odd bound state we must drop the minus sign in Eq. (13b).

Repeating the analysis of Eqs (7-9) we find in the limit $k \rightarrow 0, \kappa \rightarrow 0$ when the antiparticle is incident on the potential well $V = -U_c(x)$ with arbitrarily small momentum that

$$R_-(0) = 0 \quad T_-(0) = 1 \quad (14)$$

where $R_- = |r_-|^2, T_- = |t_-|^2$

So we see that in the Dirac equation there are two analogues of the Schrödinger result: one for zero momentum particles incident on a potential well which supports a zero momentum resonance and one for zero momentum particles incident on a supercritical potential well.

We now can obtain our main result. The Dirac equation (1) is invariant under charge conjugation: that is to say under the transformation

$$E \rightarrow -E \quad V \rightarrow -V \quad f \rightarrow g \quad g \rightarrow f \quad (15)$$

From Eq (14) we know that an antiparticle of energy $E = -\sqrt{m^2 + k^2}$ incident on the supercritical potential well $V_c(x) = -U_c(x)$ will satisfy $T_-(0) = 1$, that is to say

²In Ref [15] we adopt a more general approach to obtain the results of this letter thereby avoiding the use of $t(0) \neq 0$:

at arbitrarily small momentum it will have a vanishingly small reflection coefficient. Eq. (14) then shows that if we replace the antiparticle of energy $E = -\sqrt{m^2 + k^2}$ incident on the supercritical potential well by a particle of energy $E = \sqrt{m^2 + k^2}$ incident on the corresponding potential barrier $V(x) = +U_c(x)$ the particle will still have a transmission resonance at zero momentum, even though now the potential well has been replaced by a potential barrier. We thus obtain the theorem that where an even potential well of finite range is strong enough to contain a supercritical state, then a particle of arbitrarily small momentum will be able to tunnel right through the potential barrier created by inverting the well without reflection. This result was noticed a few years ago for the particular case of square barriers [13], and one of us (PK) has shown numerically that it was also true for Gaussian and Saxon-Woods potential barriers [18]. In the Appendix we show the behaviour of the upper and lower components of the wave function for particle scattering at zero momentum by a square and Gaussian barrier when the corresponding potential wells are supercritical.

Conclusions

In his original work Klein [7] discovered that a Dirac particle could tunnel through an arbitrarily high potential. The generic phenomenon whereby fermions can tunnel through barriers without exponential suppression we have called ‘‘Klein Tunnelling’’ [19]. The result of this letter shows that Klein tunnelling is a general feature of the Dirac equation: any potential well strong enough to support a supercritical state when inverted becomes a potential barrier which a fermion of arbitrarily low momentum can tunnel through without reflection. We do not claim here that any transmission resonance at zero momentum must correspond to supercriticality, only that supercriticality leads to a transmission resonance through a potential barrier at zero momentum. In another paper [15] we shall consider the question of the conditions on a potential for it to possess a zero momentum transmission resonance more generally. In three dimensions Hall and one of us (ND) [20] have recently demonstrated that maximal Klein tunnelling is also associated with supercriticality.

The potential step that Klein considered has pathological properties [19]. Nevertheless our result confirms that according to the Dirac equation a particle of low momentum can tunnel through an arbitrarily high smooth potential of finite range. The reason is straightforward: hole states can propagate under the potential barrier. In terms of the particle kinetic energy T under the barrier $T = E - V - m = -m - \sqrt{m^2 + q^2}$ where q is the momentum of the hole so if $T \leq -2m$, hole states can propagate without exponential suppression. $T \leq -2m$ thus corresponds to penetrating under the barrier to distances $|x| < |x_K|$ where $V(x_K) = E + m \geq 2m$ [20].

Appendix

We illustrate the result above for the special cases of

(i) a square barrier and (ii) a Gaussian barrier. First consider the square well potential $V = -U(x)$ where $U(x) = U$ for $|x| < a$ and $U(x) = 0$ for $|x| > a$. Then an unnormalised even wave function inside the well [13] has the form

$$\psi(x) = \begin{pmatrix} (E + U + m) \cos px \\ p \sin px \end{pmatrix} \quad |x| \leq a \quad (16)$$

where the internal momentum p is given by $(E + U)^2 = m^2 + p^2$. For supercriticality where $E = -m$ we require the phase condition $pa = N\pi/2$ where N is an integer [13]. The first supercritical state is thus given by $p = p_c = \pi/2a$ and correspondingly the critical potential is $V(x) = -U_c$ $|x| \leq a$, where $U_c = m + \sqrt{m^2 + \pi^2/4a^2}$. At supercriticality the wave function is thus given by

$$\psi(x) = \begin{pmatrix} 0 \\ 2m \end{pmatrix}, \quad x < -a \quad (17a)$$

$$\psi(x) = -2m \begin{pmatrix} b \cos(\pi x/2a) \\ \sin(\pi x/2a) \end{pmatrix}, \quad |x| \leq a \quad (17b)$$

$$\psi(x) = -\begin{pmatrix} 0 \\ 2m \end{pmatrix}, \quad x > a \quad (17c)$$

where $b = 2aU_c/\pi$.

Now consider a particle of arbitrarily small momentum incident on the square barrier $V(x) = U_c$ $|x| < a$; $V(x) = 0$ $|x| > a$. Eq (15) shows that the wave function is obtained by interchanging the top and bottom components of Eq (17) thereby giving the transmission resonance

$$\psi(x) = \begin{pmatrix} 2m \\ 0 \end{pmatrix}, \quad x < -a \quad (18a)$$

$$\psi(x) = -2m \begin{pmatrix} \sin(\pi x/2a) \\ b \cos(\pi x/2a) \end{pmatrix}, \quad |x| \leq a \quad (18b)$$

$$\psi(x) = -\begin{pmatrix} 2m \\ 0 \end{pmatrix}, \quad x > a \quad (18c)$$

and the components of the wave function are shown in Fig.1.

One of us (PK) has also solved the Dirac equation numerically for a Gaussian potential well and barrier where $U(x) = U \exp(-x^2/a^2)$ [18]. In Fig. 2 we show the components of the wave function for a particle of arbitrarily small momentum incident on a supercritical Gaussian barrier where $U = U_c = 3.26m$ for $ma = 1$ (cf. $U_c = m + \sqrt{m^2 + \pi^2/4a^2} = 2.86m$ for $ma = 1$ for a square barrier). Again there is a transmission resonance demonstrating complete penetration of the barrier.

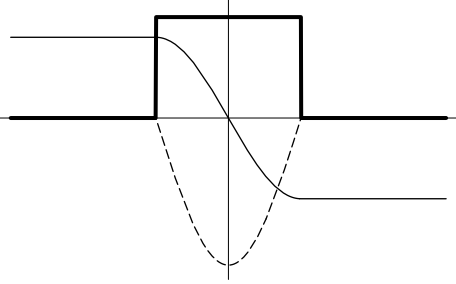


FIG. 1. The zero momentum wave function for the square barrier $V = U_c(x)$, depicted by the heavy line. The solid line is the upper component and the dashed line is the lower component.

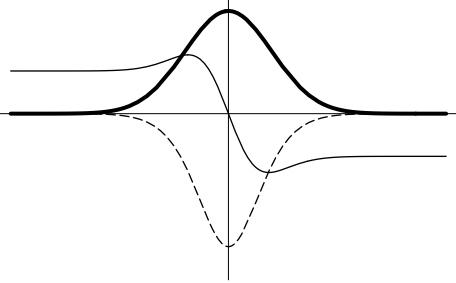


FIG. 2. The zero momentum wave function for the Gaussian barrier $V = U_c \exp(-m^2 x^2)$, depicted by the heavy line. The solid line is the upper component and the dashed line is the lower component

While the wave functions in this case have a similar form to those for the square barrier, note the two turning points which occur in the top component of the Gaussian wave function. These correspond to the points $\pm x_K$ where $V(x_K) = E + m = 2m$ at zero momentum. Hole states can propagate under the potential without exponential suppression from $-x_K$ to $+x_K$ thus demonstrating Klein tunnelling. Note also that the condition for hole states to propagate under a potential of finite range is $V > 2m$ which will in general not be sufficient for supercriticality (we have seen for a square barrier of range a with $ma = 1$ that $V_c = 2.86m$). So Klein tunnelling should exist even for subcritical potentials as was pointed out by Jensen et al [21].

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